International Journal of Modern Physics E

Isospin mixing of isospin-projected Slater determinants: formalism and preliminary applications

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Received (received date)
Revised (revised date)

We report on the development of a new theoretical tool that allows for isospin projection of Slater determinants and we present its first applications. In particular, we determine the isospin mixing in ground states of $N = Z$ nuclei and discuss its dependence on the size of the harmonic-oscillator basis used in the calculations. We also discuss the unphysical contribution to the isospin mixing caused by the spurious isospin-symmetry breaking inherent to the mean-field approach. We show that these contributions may be as large as 30% of the value of the isospin-mixing parameter.

1. Introduction

Self-consistent mean-field (MF) approach is practically the only formalism allowing for large-scale no-core computations in heavy open-shell nuclei with many valence particles. Inherent to the MF approach is the mechanism of spontaneous symmetry breaking, which is essentially the only way to allow for incorporating a significant part of many-body correlations into a single intrinsic (symmetry-breaking) Slater determinant. However, unlike in the cases of rotational or translational symmetry-breaking schemes, violation of the isobaric symmetry has two distinctively different sources. The unwanted or *unphysical* source pertains directly to the MF approximation[1,2,3,4]. It manifests itself very clearly in the ground-state wave functions calculated by using isospin-invariant interactions, like Skyrme or Gogny forces, with Coulomb force neglected. Indeed, such calculations manifestly break the isospin symmetry in all but the $N = Z$ systems, simply because the self-consistent proton and neutron wave functions are then different. The second source of the isospin-symmetry violation is of strictly *physical* nature and is caused mostly by the Coulomb field and, to a much lesser extent, by strong-force isospin-non-invariant components.

Hereby, we report on the development of a new theoretical tool that allows for isospin projection (after variation) of Slater determinants. It has been implemented within the Hartree-Fock code HFODD[5,6]. First, the Slater determinants are deter-

mined in a standard way by minimizing the Skyrme functional plus the Coulomb energy. Both direct and exchange terms of the Coulomb energy are calculated exactly. We allow for arbitrary spatial deformations of these intrinsic states. Second, the isospin-projected components are determined, and third, they are mixed so as to rediagonalize the total Skyrme-plus-Coulomb Hamiltonian.

Such a three-step procedure allows, respectively, for (i) taking into account the competition between the nuclear and Coulomb interactions in building up the single Slater determinant, which is becoming 'deformed' in the isospace, (ii) restoring the isospin symmetry, and (iii) letting the nuclear and Coulomb interactions pick the correct mixtures of symmetry-restored eigenstates of the isospin.

In the present study, we briefly overview the main theoretical building blocks of the formalism (Sect. 2) and discuss preliminary applications. In particular, we give results for the isospin-mixing parameters (α_C) calculated in the ground states of $N = Z$ nuclei (Sect. 3). The ultimate goal will be to perform simultaneous isospin and angular momentum[7,8] projections and to systematically calculate the isospin-symmetry breaking corrections to the Fermi matrix element (δ_C) for the set of nuclei undergoing the superallowed $0^+ \to 0^+$ Fermi beta decay[9,10].

2. Theoretical formalism: isospin restoration and Coulomb rediagonalization scheme

The first step and the starting point of our approach is the determination of the isospin-symmetry-broken single-particle (s.p.) Slater determinant $|\mathrm{HF}\rangle$ calculated by using the Hartree-Fock (HF) theory including the isospin-invariant Skyrme ($\hat{V}^S$) and the isospin-symmetry-breaking Coulomb ($\hat{V}^C$) interactions:

$$\hat{H} = \hat{H}^S + \hat{V}^C \quad \text{where} \quad \hat{H}^S = \hat{T} + \hat{V}^S. \tag{1}$$

The isospace-deformed state $|\mathrm{HF}\rangle$ admixes higher isospin components $T \geq |T_z|$:

$$|\mathrm{HF}\rangle = \sum_{T \geq |T_z|} b_{T,T_z} |\eta; T, T_z\rangle, \tag{2}$$

where T and T_z are the total isospin and its third component, respectively, η labels all other quantum numbers pertaining to the $|\mathrm{HF}\rangle$ state, and the coefficients b_{T,T_z} are such that $\sum_{T \geq |T_z|} |b_{T,T_z}|^2 = 1$.

In the second step we create the good-isospin states $|\eta; T, T_z\rangle$ by projecting them out from the Slater determinant $|\mathrm{HF}\rangle$:

$$|\eta; T, T_z\rangle = \frac{1}{b_{T,T_z}} \hat{P}^T_{T_z T_z} |\mathrm{HF}\rangle. \tag{3}$$

In the following, we denote the mixing coefficients b_{T,T_z} and average energies E^{BR}_{T,T_z}:

$$|b_{T,T_z}|^2 = \langle \mathrm{HF}|\hat{P}^T_{T_z T_z}|\mathrm{HF}\rangle \quad , \quad E^{\mathrm{BR}}_{T,T_z} = \langle \eta; T, T_z|\hat{H}|\eta; T, T_z\rangle, \tag{4}$$

as being obtained *before rediagonalization*. In the above formulae, $\hat{P}^T_{T_z T_z}$ denotes the conventional[11] SO(3) projection operator reduced to one dimension due to the

T_z quantum number conservation, that is:

$$\hat{P}^T_{T_zT_z} = \frac{2T+1}{2}\int_0^\pi d\beta \sin\beta d^T_{T_zT_z}(\beta)\hat{R}(\beta), \tag{5}$$

where $\hat{R}(\beta) = e^{-i\beta\hat{T}_y}$ denotes active-rotation operator by the Euler angle β in the isospace and $d^T_{T_zT_z}(\beta)$ is the Wigner d-function[12].

In the third step we mix the projected states,

$$|\eta; n, T_z\rangle = \sum_{T\geq|T_z|} a^n_{T,T_z}|\eta; T, T_z\rangle, \tag{6}$$

and determine the mixing coefficients a^n_{T,T_z} by diagonalizing Hamiltonian (1) in the space of projected states,

$$\sum_{T'\geq|T_z|}\langle\eta; T, T_z|\hat{H}|\eta; T', T_z\rangle a^n_{T',T_z} = E^{\rm AR}_{n,T_z}a^n_{T,T_z}, \tag{7}$$

where n enumerates the obtained eigenstates. In the following, we denote the mixing coefficients a^n_{T,T_z} and eigenenergies $E^{\rm AR}_{n,T_z}$ as being obtained *after rediagonalization*. The lowest-energy solution, for $n = 1$, corresponds to the isospin mixing in the ground state.

The Skyrme Hamiltonian, $\hat{H}^S$, is an isoscalar operator; hence, it contributes only to the diagonal matrix elements of the Hamiltonian (1), $\langle\eta; T, T_z|\hat{H}^S|\eta; T, T_z\rangle$, which can be obtained from:

$$\langle{\rm HF}|\hat{H}^S\hat{P}^T_{T_zT_z}|{\rm HF}\rangle = \int_0^\pi d\beta \sin\beta\, d^T_{T_zT_z}(\beta)\langle{\rm HF}|\hat{H}^S\hat{R}(\beta)|{\rm HF}\rangle. \tag{8}$$

Similarly, calculation of the diagonal and non-diagonal matrix elements of the Coulomb interaction, $\langle\eta; T, T_z|\hat{V}^C|\eta; T', T_z\rangle$, can be efficiently performed after decomposing $\hat{V}^C$ into the isoscalar, $\hat{V}^C_{00}$, isovector, $\hat{V}^C_{10}$, and isotensor, $\hat{V}^C_{20}$, components, and by making use of the SO(3) transformation rules for the spherical tensors under rotations in the isospace[12]. In the particular case of one-dimensional projection we deal with in this work, all matrix elements of axial spherical tensors reduce to one-dimensional integrals over the Euler angle β:

$$\begin{aligned}\langle{\rm HF}|\hat{P}^T_{T_zT_z}\hat{V}^C_{\lambda 0}\hat{P}^{T'}_{T_zT_z}|{\rm HF}\rangle \;=\; & C^{TT_z}_{T'T_z\;\lambda 0}\sum_{\mu'=-\lambda}^{\lambda} C^{TT_z}_{T'T'_z\;\lambda\mu'} \\ & \frac{2T'+1}{2}\int_0^\pi d\beta\;\sin\beta\, d^{T'}_{T'_z,T_z}(\beta)\,\langle{\rm HF}|\hat{V}^C_{\lambda\mu'}\hat{R}(\beta)|{\rm HF}\rangle,\end{aligned} \tag{9}$$

where $T'_z = T_z - \mu'$ and $C^{TT_z}_{T'T'_z\;\lambda\mu}$ denote standard Clebsch-Gordan coefficients. The Skyrme-Hamiltonian and Coulomb-interaction kernels, $\langle{\rm HF}|\hat{H}^S\hat{R}(\beta)|{\rm HF}\rangle$ and $\langle{\rm HF}|\hat{V}^C\hat{R}(\beta)|{\rm HF}\rangle$, respectively, can be evaluated by using expressions for the standard diagonal kernels[13] ($\beta = 0$) and replacing there the isoscalar and isovector densities and currents with the so-called transition densities and currents. Exact direct and exchange kernels of the Coulomb interaction can be evaluated by using methods outlined in Refs.[14,15,16].

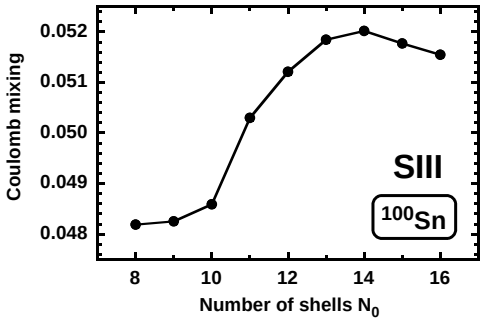

Fig. 1. The isospin-mixing parameter α_C calculated in ^{100}Sn (after rediagonalization) as a function of the number of the HO shells N_0. The results were obtained by using the SIII[17] Skyrme parameterization.

3. Numerical applications: the isospin mixing and the isospin-projected energies in N=Z nuclei

The isospin-mixing parameter, calculated before and after rediagonalization, is defined as $\alpha_C = 1 - |b_{|T_z|,T_z}|^2$ and $\alpha_C = 1 - |a^{n=1}_{|T_z|,T_z}|^2$, respectively. Its theoretical accuracy depends on different factors, and in particular, on the size of the spherical harmonic-oscillator (HO) basis used in the calculations. A choice of the number of the HO shells N_0 included in such calculations is always a result of a trade-off between the accuracy and the CPU-time efficiency. In this respect, a bottle-neck in our calculation scheme is the exact treatment of the exchange Coulomb contribution, which makes calculations prohibitively time consuming for $N_0 > 16$.

Dependence of the isospin-mixing parameter on N_0 is depicted in Fig. 1. The figure shows α_C in ^{100}Sn, calculated after rediagonalization, by using the SIII Skyrme parameterization of Ref.[17]. In the expanded scale of the figure, a significant variation of the mixing parameter with N_0 is clearly seen. Unfortunately, the mixing parameter α_C does not stabilize at $N_0 = 16$. Hence, by using the present method, α_C cannot be calculated with the absolute precision greater than ± 0.002, or with the relative precision grater than $\pm 4\%$. However, our studies show that the inaccuracy in evaluating α_C due to the basis cut-off appears to be much smaller than the uncertainty related to the Skyrme force parameterization[18].

Fig. 2 shows the total binding energies versus N_0, calculated for doubly magic nuclei: ^{16}O, ^{40}Ca, ^{56}Ni, and ^{100}Sn. This set of calculations was performed by using the SII Skyrme force parameterization[17]. The curves labeled by black squares depict the projected energies $E^{\rm BR}_{T,T_z}$ (4), calculated before rediagonalization, and those marked by triangles show the total binding energies $E^{\rm AR}_{n=1,T_z}$ (7), obtained after rediagonalization of the total Hamiltonian in the isospin-projected basis. The figure shows that (*i*) the Coulomb rediagonalization effect increases with increasing Z as anticipated, and that (*ii*) the choice of $N_0 = 12$ HO shells provides a reasonable estimate for the total binding energy even for ^{100}Sn. Hence, all calculations

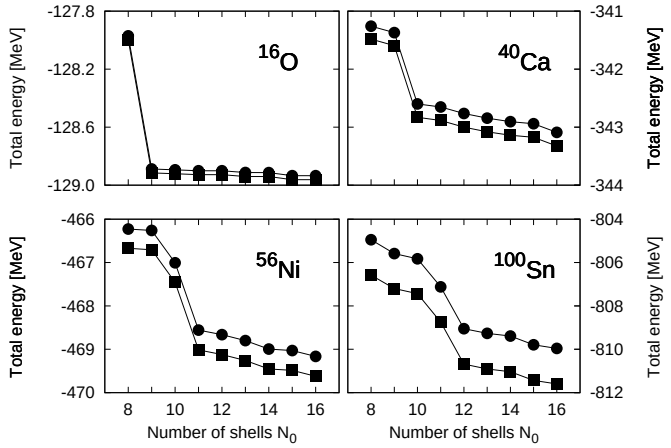

Fig. 2. Total binding energies in ^{16}O, ^{40}Ca, ^{56}Ni, and ^{100}Sn as a functions of the number of the HO shells N_0. Calculations were performed by using the SII Skyrme force[17]. Dots and squares label the binding energies calculated before and after rediagonalization, respectively.

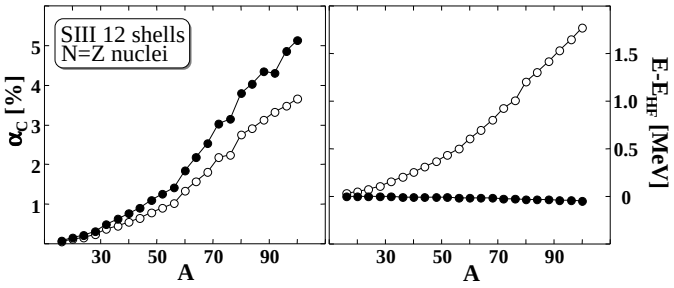

Fig. 3. The isospin mixing (left) and the difference between the total binding energy and the HF energy (right) in $N = Z$ nuclei, calculated for the SIII Skyrme force and $N_0 = 12$ HO shells. The results shown by open and full dots represent variants of the calculation before and after rediagonalization, respectively.

presented below are done for $N_0 = 12$.

Fig. 3a shows the isospin mixing in $N = Z$ nuclei as a function of the mass number A. Results obtained before and after rediagonalization are shown by open and full dots, respectively. In both variants of the calculations, the isospin mixing shows a gradual increase as a function of A. It increases from a fraction of a percent in ^{16}O to about 4%–5%, depending on the variant of the calculation. Note that the results obtained before rediagonalization follow closely those obtained in Ref.[19].

The isospin mixing obtained after removing the spurious mean-field component through the Coulomb rediagonalization is systematically larger than the one obtained within the HF method followed by the exact isospin projection. This result

confirms that the mean-field breaks the isospin symmetry in such a way that it counterbalances the external symmetry breaking mechanism caused by the Coulomb field. Nevertheless, as clearly seen in Fig. 3b, the HF energy is astonishingly close to the total energy obtained after the Coulomb rediagonalization.

4. Summary

In the present study, we presented a new theoretical tool that allowed for isospin projection of Slater determinants and we discussed first applications of the formalism to calculate the isospin-mixing parameters α_C and total binding energies in $N = Z$ nuclei. In particular, we discussed the basis-size dependence of α_C and we showed that the basis truncation may introduce about $\pm 4\%$ uncertainty in α_C.

We also discussed the role and magnitude of the spurious isospin-symmetry-violating response of the self-consistent mean field against the physical symmetry-breaking effects of the Coulomb field. We showed that even in $N = Z$ nuclei, the self-consistent mean-field may induce unphysical isospin mixing that reduces α_C by as much as 30% in ^{100}Sn. This unphysical mechanism is due to the very variational nature of the self-consistent mean-field scheme, which introduces its own isospin-symmetry breaking field and partly counterbalances the repulsive symmetry-breaking Coulomb field so as to minimize the total binding energy. Nevertheless, our calculations show that the HF binding energies follow extremely closely those obtained by rediagonalizing the Hamiltonian within the set of isospin-projected states.

This work was supported in part by the Polish Ministry of Science under Contract No. N N202 328234 and by the Academy of Finland and University of Jyväskylä within the FIDIPRO programme.

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